Computing spectra, Grassmannians and symmetry

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Spectral problems

Elliptic operator on $\mathbb{R} \times \mathbb{T}$:

$$H := B\,(\partial_x^2 + \partial_y^2) + d\,\partial_x + V(x,y).$$

Eigenvalue problem:

$$(H - \lambda)q = O \qquad \Leftrightarrow \qquad (\partial_x - A)Y = O$$

where $\partial - A : H^1(\mathbb{R};\mathbb{H}) \to L^2(\mathbb{R};\mathbb{H})$.

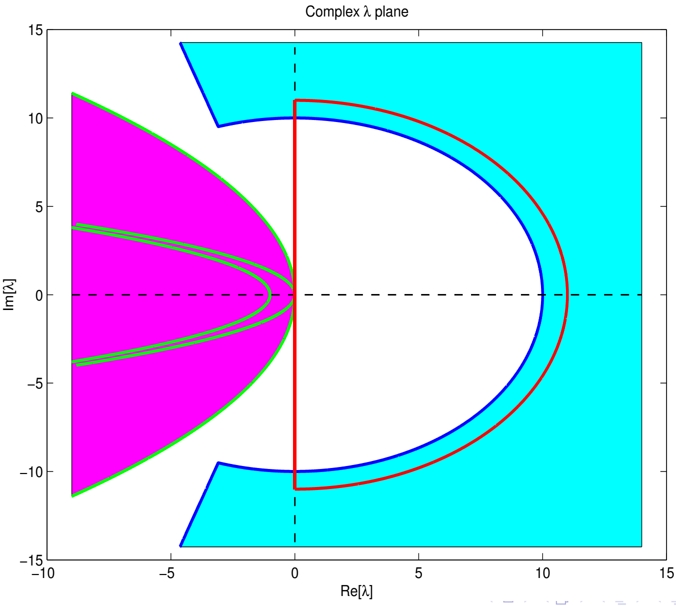
First case: $\mathbb{H} = \mathbb{C}^n$, no y dependence, ker and coker finite.

Numerical resolution of pure point spectrum

Main solution approaches:

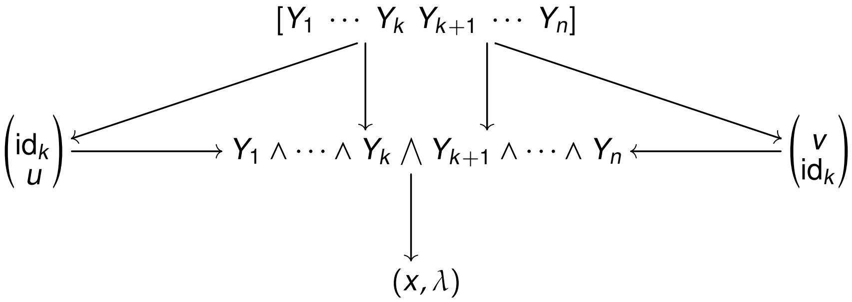
- *Projection and iteration;*
- *Shooting and matching;*
- *Perturbative: operator determinants.*

Spectrum



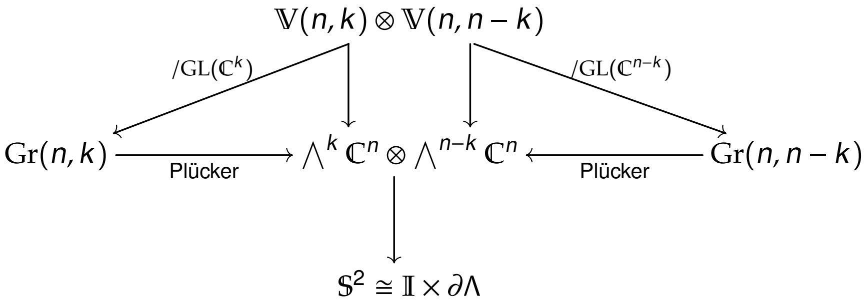
Shooting and matching

Region: $\Lambda \subseteq \{\lambda : \partial - A \in \mathrm{Fred}_0\}$.

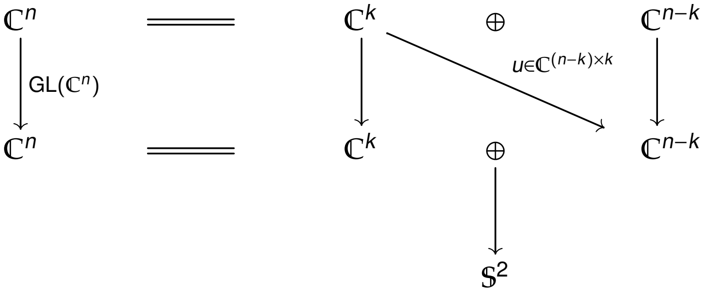


(Humpherys & Zumbrun 2006)

Determinant line bundle



Polarization of $\mathbb{C}^n$



Grassmannian flow

Evolutionary problem for $\partial - A$:

$$\partial \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}$$

Suppose $\exists$ map $u\colon\, q \mapsto p$.

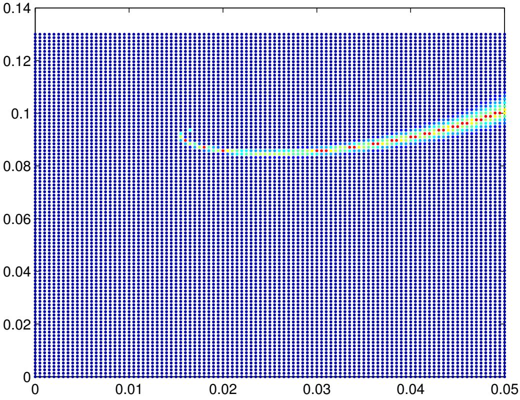
$$\Longrightarrow \qquad \partial q = (a + bu)\, q$$

$$\Longrightarrow \qquad \begin{aligned} (\partial u)\, q &= \partial(uq) - u\,\partial q \\ &= c\, q + du\, q - u(a + bu)\, q \end{aligned}$$

$$\Leftrightarrow \qquad \partial u = c + du - u(a + bu)$$

Singularities

Ledoux & M. 2009:



Qu: where do eigenvalues evolute from?

Infinite dimensional case

Second case: $\mathbb{H} = L^2(\mathbb{T};\mathbb{C}^n) \cong (\ell^2)^n$; same Λ: $\partial - A \in \text{Fred}_0$.

$$q(x,y) \rightsquigarrow \hat{q}(x,k)$$

Evolutionary problem:

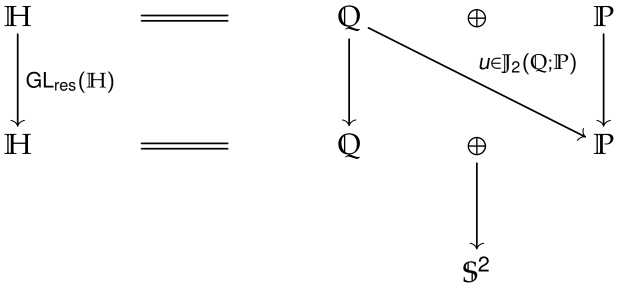
$$(\partial - A)\begin{pmatrix}\hat{q}\\ \hat{p}\end{pmatrix} = O$$

where

$$A\begin{pmatrix}\hat{q}\\ \hat{p}\end{pmatrix} = \begin{pmatrix} O & \text{id} \\ B^{-1}(\lambda + D - \hat{V}\star) & -B^{-1}d\end{pmatrix}\begin{pmatrix}\hat{q}\\ \hat{p}\end{pmatrix}$$

(Sanstede & Scheel 2008: “Relative Morse indices, ...”)

Polarization of $\mathbb{H}$



(Pressley & Segal 1986)

Superpotential

Recap. $u \in C^\infty\big(\mathbb{I}; \mathbb{J}_2(\mathbb{Q}; \mathbb{P})\big)$ and $v \in C^\infty\big(\mathbb{I}; \mathbb{J}_2(\mathbb{P}; \mathbb{Q})\big)$ satisfy

$$\partial u = c + du - u(a + bu) \qquad \text{and} \qquad \partial v = b + av - v(d + cv),$$

Define $U \in C^\infty\big(\mathbb{I}; \mathrm{GL}_{\mathrm{res}}(\mathbb{H})\big)$ by

$$U := \begin{pmatrix} \mathrm{id} & v \\ u & \mathrm{id} \end{pmatrix}.$$

Then

$$U^{-1}(\partial - A)\, U = \begin{pmatrix} \partial - (a + bu) & O \\ O & \partial - (d + cv). \end{pmatrix}$$

(Beck & M. 2013)

Quillen determinant bundle

$$\bigwedge^k \ker(H)^* \otimes \bigwedge^{k'} \operatorname{coker}(H)$$

$$\downarrow$$

$$H \in \mathrm{Fred}_0$$

Furutani 2004 $\implies$ isom. to Fredholm Det line bundle

Synonyms

Carrying the same information for $d \geqslant 1$ are:

- Evans matrix/augmented unstable bundle;
- Miss-distance function;
- Titchmarsh–Weyl matrix-function;
- Scatter/Transmission matrix;
- Dirichlet-to-Neumann map;
- Fredholm determinant line bundle;
- Quillen determinant line bundle;
- Grassmannian (Fredholm) flow.

References

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2. N.D. Aparicio, S.J.A. Malham and M. Oliver, *Numerical evaluation of the Evans function by Magnus integration*, BIT 45 (2005), pp. 219–258.
3. N.J. Balmforth, R.V. Craster and S.J.A. Malham, *Unsteady fronts in an autocatalytic system*, Proc. R. Soc. Lond A. 455 (1999), pp. 1401–1433.
4. J. Humpherys and K. Zumbrun, *An efficient shooting algorithm for Evans function calculations in large systems*, Physica D 220 (2006), pp. 116–126.

References II

1. V. Ledoux, M. Van Daele and G. Vanden Berghe, *A numerical procedure to solve the multichannel Schrödinger eigenvalue problem*, Comp. Phys. Commun. 176 (2007). pp. 191-199.
2. V. Ledoux, S.J.A. Malham and V. Thümmler, *Grassmannian spectral shooting*, Mathematics of Computation 79 (2010), pp. 1585–1619.
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Setup

On $\mathbb{R}$: $\quad B\,\partial_{xx}U + c\,\partial_x U + \mathrm{D}F(U_c)U = \lambda U$

$$\Leftrightarrow \qquad \begin{aligned} \partial_x U &= P, \\ \partial_x P &= B^{-1}\big(\lambda - \mathrm{D}F(U_c)\big)U - cB^{-1}P. \end{aligned}$$

$$\Leftrightarrow \qquad Y' = A(x;\lambda)\,Y.$$

For $\lambda \in \mathbb{C}$: matching condition

$$\begin{aligned} D(\lambda) &:= \mathrm{e}^{\int_0^x \mathrm{Tr}A(\xi;\lambda)\,\mathrm{d}\xi} \det\big(Y_1^- \ \cdots \ Y_k^- \ Y_{k+1}^+ \ \cdots \ Y_n^+\big) \\ &= \mathrm{e}^{\int_0^x \mathrm{Tr}A(\xi;\lambda)\,\mathrm{d}\xi} \det\big(Y^- \ \ Y^+\big) \end{aligned}$$

Numerical issues

- Computational domain.
- Different exponential growth rates.
- Polynomial complexity.
- Flow singularities?!
- Where to match?
- Retaining analyticity?
- How to project transversely.
- How to approximate the Fredholm Grassmannian flow.

Stiefel and Grassmann manifolds

- Stiefel manifold:

$$\mathbb{V}(n,k) = \{k\text{-frames centred at the origin}\}.$$

- Grassmann manifold:

$$\mathrm{Gr}(n,k) = \{k\text{-dimensional subspaces of } \mathbb{C}^n\}.$$

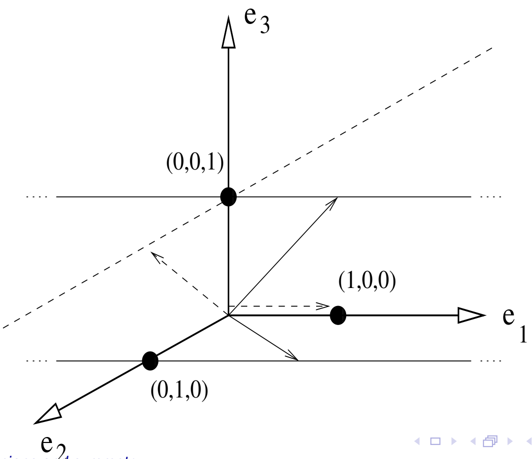
- Fibre bundle:

$$\pi : \mathbb{V}(n,k) \to \mathrm{Gr}(n,k) \cong \mathbb{V}(n,k)/\mathrm{GL}(k)$$
$$\pi : k\text{-frame} \mapsto \text{spanning } k\text{-plane}$$

Representation

Example: $\mathrm{Gr}(3,2)$

$$\begin{pmatrix} * & 1 & 0 \\ * & 0 & 1 \end{pmatrix}; \qquad \begin{pmatrix} 1 & 0 & 0 \\ 0 & * & 1 \end{pmatrix}; \qquad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$



Representation II

$\pi\colon Y = y_{\mathfrak{i}^\circ} u \mapsto y_{\mathfrak{i}^\circ}$

Example coordinate patch:

$$y_{\mathfrak{i}^\circ} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ \hat{y}_{k+1,1} & \hat{y}_{k+1,2} & \cdots & \hat{y}_{k+1,k} \\ \hat{y}_{k+2,1} & \hat{y}_{k+2,2} & \cdots & \hat{y}_{k+2,k} \\ \vdots & \vdots & \ddots & \vdots \\ \hat{y}_{n,1} & \hat{y}_{n,2} & \cdots & \hat{y}_{n,k} \end{pmatrix}.$$

Local chart $\mathbb{U}_{\mathfrak{i}} \to \mathbb{C}^{(n-k)k}$ given by $y_{\mathfrak{i}^\circ} \mapsto \hat{y}$.

Grassmannian flows

$$Y' = A(x, Y)\, Y$$

Substitute decomposition $Y = y_{\mathfrak{i}^\circ} u$:

$$y_{\mathfrak{i}^\circ}' u + y_{\mathfrak{i}^\circ} u' = (A_{\mathfrak{i}} + A_{\mathfrak{i}^\circ} \hat{y})\, u$$

Project onto $\mathfrak{i}^\circ$th and $\mathfrak{i}$th rows:

$$\hat{y}' = c + d\, \hat{y} - \hat{y}(a + b\, \hat{y}) \qquad \text{and} \qquad u' = (a + b\, \hat{y})\, u$$

where $a = A_{\mathfrak{i}\times\mathfrak{i}}$, $b = A_{\mathfrak{i}\times\mathfrak{i}^\circ}$, $c = A_{\mathfrak{i}^\circ\times\mathfrak{i}}$ and $d = A_{\mathfrak{i}^\circ\times\mathfrak{i}^\circ}$.

Schubert cycles

- $\mathrm{Gr}(4,2)$ Schubert cells are:

$$C_{\{1,2\}}: \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad C_{\{1,3\}}: \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & * & 1 & 0 \end{pmatrix} \quad C_{\{1,4\}}: \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & * & * & 1 \end{pmatrix}$$

$$C_{\{2,3\}}: \begin{pmatrix} * & 1 & 0 & 0 \\ * & 0 & 1 & 0 \end{pmatrix} \quad C_{\{2,4\}}: \begin{pmatrix} * & 1 & 0 & 0 \\ * & 0 & * & 1 \end{pmatrix} \quad C_{\{3,4\}}: \begin{pmatrix} * & * & 1 & 0 \\ * & * & 0 & 1 \end{pmatrix}$$

- Schubert cycles $\Leftrightarrow$ Cohomological ring $\Leftrightarrow$ Schur polynomials
- Fibre bundle over $\mathbb{S}^2$ with fibres $\mathrm{Gr}(n,k)$
- Chern character? From tautological Grassmann bundle?
- Computational efficiencies?

Grassmannian Gaussian elimination method (GGEM)

$$
\begin{array}{ccccc}
\mathbb{C}^{(n-k)k} & \xrightarrow{\text{chartmap}^{-1}} & \mathbb{U}_{\mathfrak{i}} & \xrightarrow{\text{id}} & \mathbb{V}(n,k) \\
\Big\downarrow \textit{Riccati} & & \Big\downarrow \textit{GGEM} & & \Big\downarrow \textit{RK} \\
\mathbb{C}^{(n-k)k} & \xleftarrow[\text{newchart}]{} & \mathbb{U}_{\mathfrak{i}'} & \xleftarrow[\text{QOGE}]{} & \mathbb{V}(n,k)
\end{array}
$$

Quasi-optimal Gaussian elimination (QOGE)

GE with *free* stepwise max pivot, generates:

$$\begin{pmatrix} * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ * & * & * & * & \cdots & * \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ * & * & * & * & \cdots & * \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ * & * & * & * & \cdots & * \\ 0 & 0 & 0 & 0 & \cdots & 1 \\ * & * & * & * & \cdots & * \end{pmatrix}$$

Applications (planar fronts)

- $D(\lambda) := \mathrm{e}^{-\int_0^x \mathrm{Tr} A(\xi;\lambda)\,\mathrm{d}\xi} \det\big(Y^-(x;\lambda)\ \ Y^+(x;\lambda)\big)$
- $\det\big(Y^-\ Y^+\big) = \det\big(y_{\mathrm{i}_-^\circ}\quad y_{\mathrm{i}_+^\circ}\big) \cdot \det\, u_{\mathrm{i}_-} \cdot \det\, u_{\mathrm{i}_+}$
- $D(\lambda; x_*) := \det\big(y_{\mathrm{i}_-^\circ}\quad y_{\mathrm{i}_+^\circ}\big)$
- Record any patch change to retain analyticity.

Boussinesq system

PDE: $u_{tt} = (1 - c^2)\, u_{xx} + 2c\, u_{xt} - u_{xxxx} - (u^2)_{xx}$.

Solitary waves with sech^2 profile.

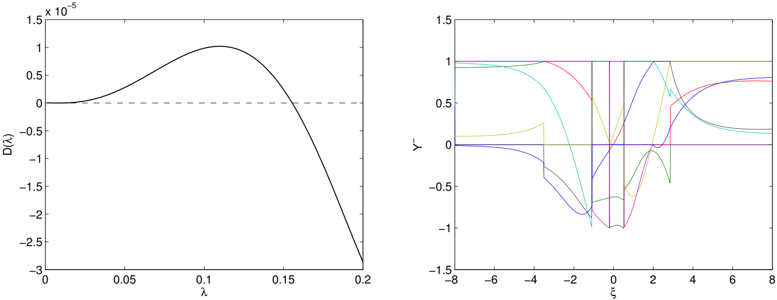


Figure : Evans function for $c = 1/4$ with GGEM-RK and $x_* = 8$ (left panel). Entries of $y_{\hat{\imath}}$ for $\lambda = 0.15543141$ (right panel).

Boussinesq: error vs matching point

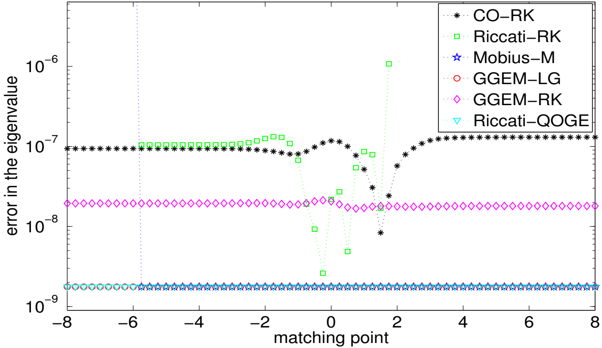


Figure : Error in the eigenvalue for different choices of the matching point: $N = 512$.

Autocatalytic fronts

$$\partial_t u = \delta \Delta u + c \partial_x u - u v^m,$$
$$\partial_t v = \Delta v + c \partial_x v + u v^m.$$

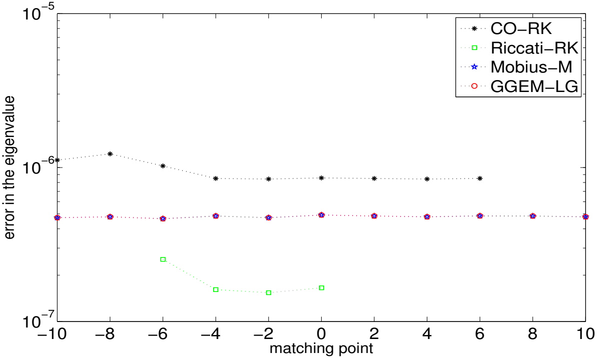


Figure : Error in the eigenvalue when $\delta = 0.1$ and $m = 9$: $N = 256$.

Transverse Fourier basis

On $\mathbb{R} \times \mathbb{T}$ we have:

$$B\Delta U + c\,\partial_x U + \mathrm{D}F(U_c)U = \lambda U.$$

On the Fourier modes $k = -K, -K+1, \ldots, K$:

$$\begin{aligned}
\partial_x \hat{U}_k &= \hat{P}_k, \\
\partial_x \hat{P}_k &= \lambda B^{-1}\hat{U}_k + (k/\tilde{L})^2 \hat{U}_k - \sum_{\nu=-K}^{K} B^{-1}\hat{D}_{k-\nu}\hat{U}_\nu - c\,B^{-1}\hat{P}_k.
\end{aligned}$$

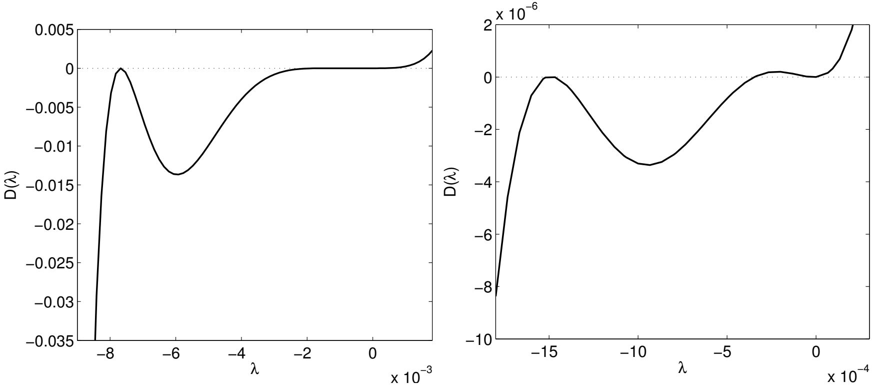
Computing travelling waves: freezing method

Substitute $U(x,y,t) = V(x-\gamma(t),y,t)$ into original PDE:

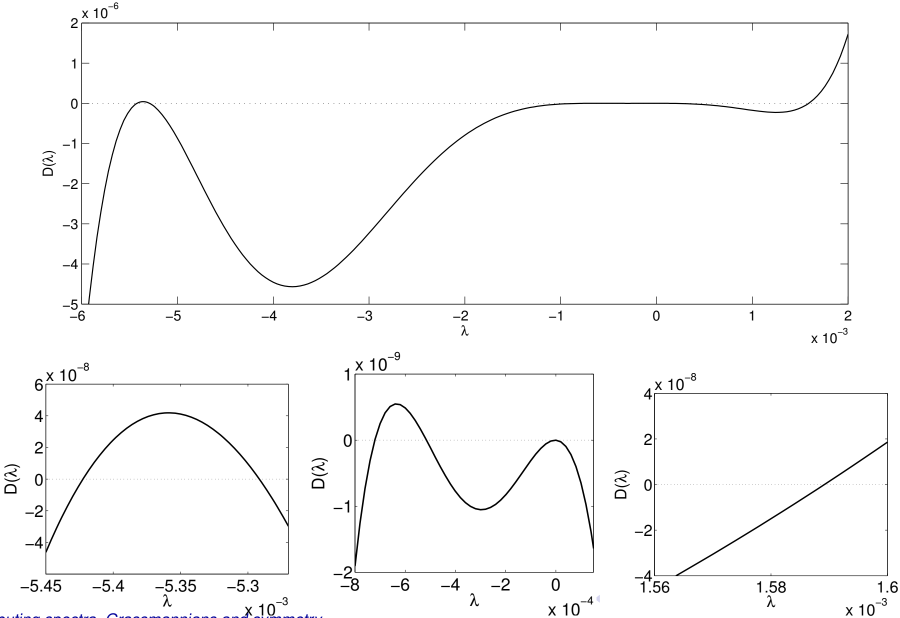
$$
\begin{aligned}
\partial_t V &= B\,\Delta V + \gamma'(t)\partial_x V + F(V), \\
0 &= \int_{\mathbb{R}\times\mathbb{T}} \Big(\partial_x \hat{V}(x,y,t)\Big)^{\mathrm{T}} \Big(\hat{V}(x,y,t) - V(x,y,t)\Big)\,\mathrm{d}x\,\mathrm{d}y.
\end{aligned}
$$

(Developed by Beyn and Thümmler.)

Wrinkled front: Evans function for $\delta = 2.5$



Wrinkled front: Evans function for $\delta = 3$



Wrinkled front: Eigenvalues for $\delta = 3$

K	Eigenvalues (Evans function)				
3	0.001609	−0.000026	−0.000781	−0.001296	−0.000670
4	0.001609	0.000002	−0.000001	−0.000519	−0.000670
5	0.001589	0.000002	−0.000001	−0.000519	−0.000720
6	0.001589	−0.000002	−0.000003	−0.000515	−0.000720
7	0.001589	−0.000002	−0.000003	−0.000515	−0.000721
8	0.001589	−0.000002	−0.000003	−0.000515	−0.000721
9	0.001589	−0.000002	−0.000003	−0.000515	−0.000721
⋮			⋮		
24	0.001589	−0.000002	−0.000003	−0.000515	−0.000721
	Eigenvalues (ARPACK)				
	0.001592	0.000000	0.000000	−0.000514	−0.000719

Wrinkled front: contour integration

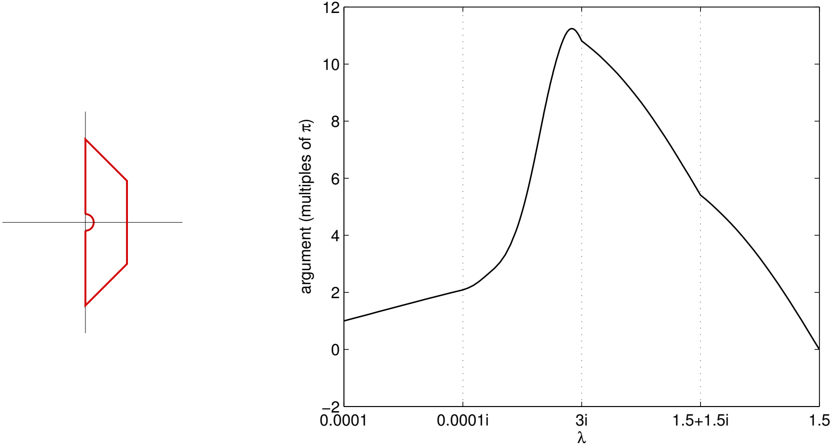


Figure : Left panel: contour. Right panel: $\arg\big(D(\lambda)\big)$ when λ transverses the top half. $\delta = 3$.

Fredholm determinant

$$
\begin{aligned}
& Y' = \Big(A_0(\lambda) + A_1(x)\Big)\, Y \\
\Leftrightarrow \qquad & \Big(\partial_x - A_0\Big) Y = A_1\, Y \\
\Leftrightarrow \qquad & \Big(\mathrm{id} - (K_{A_0} \circ A_1)\Big)\, Y = O
\end{aligned}
$$

Compute $\det_{\mathrm{F}}(\mathrm{id} + K)$ for $K = -K_{A_0} \circ A_1$.

For Hilbert space $\mathbb{H}$:

$$
\operatorname{tr} K := \sum_{i \geqslant 1} \langle \varphi_i, K\varphi_i \rangle_{\mathbb{H}} = \int_{\mathbb{R}} \operatorname{tr} G(x; x)\, \mathrm{d}x
$$

Fredholm expansion

$$\det(\mathrm{id} + K) = \sum_{m \geqslant 0} \mathrm{tr}\, K^{\wedge m}$$

where

$$\begin{aligned} \mathrm{tr}\, K^{\wedge m} &= \sum_{i_1 < \cdots < i_m} \left\langle \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_m}, K\varphi_{i_1} \wedge \ldots \wedge K\varphi_{i_m} \right\rangle_{\mathbb{H}^{\wedge m}} \\ &= \sum_{i_1 < \cdots < i_m} \det\Big[\langle \varphi_{i_p}, K\varphi_{i_q} \rangle_{\mathbb{H}}\Big]_{p,q \in \{1,\ldots,m\}} \\ &= \frac{1}{m!} \int_{\mathbb{R}^m} \det\Big[G(x_i, x_j)\Big] \,\mathrm{d}x_1 \ldots \mathrm{d}x_m \end{aligned}$$

Bornemann, apply quadrature to:

$$(\mathrm{id} + K)\, Y = f$$

Multi-dimensional shooting

The Fredholm determinant and Evans function are related:

$$\det(\mathrm{id} + K) = \frac{\det(Y^- \;\; Y^+)}{\det(Y_0^- \;\; Y_0^+)}$$

(Proved in general setting by Karambal 2011.)

Suppose $\mathbb{H} = \mathbb{H}_1 \oplus \mathbb{H}_2$: say $\mathbb{H}_1 = H^{\frac{1}{2}}(\partial\Omega)$ and $\mathbb{H}_2 = H^{-\frac{1}{2}}(\partial\Omega)$:

$$\mathrm{Gr}(\mathbb{H}) := \begin{cases} W & : \pi_1 : W \to \mathbb{H}_1 \text{ is Fredholm} \\ W & : \pi_2 : W \to \mathbb{H}_2 \text{ is Hilbert–Schmidt} \end{cases}$$

i.e. it is a Hilbert manifold modelled on $\mathbb{J}_2(\mathbb{H}_1, \mathbb{H}_2)$.